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# Health and Environmental Effects Profile for N,N-Diethylaniline

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Cincinnati, OH

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16. ABSTRACT

The Health and Environmental Effects Profile for N,N-diethylaniline was prepared by the Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH for the Office of Solid Waste and Emergency Response to support listings of hazardous constituents of a wide range of waste streams under Section 3001 of the Resource Conservation and Recovery Act (RCRA) and to provide health-related limits for emergency actions under Section 101 of the Comprehensive Environmental Response, Compensation and Liability Act (CERCLA). Both published literature and information obtained from Agency program office files were evaluated as they pertained to potential human health, aquatic life and environmental effects of hazardous waste constituents.

Quantitative estimates have been presented provided sufficient data are available. Existing data are insufficient to determine a Reference Dose (~~RfD~~) or a carcinogenic potency factor for N,N-diethylaniline.

The Reportable Quantity (RQ) value of 1, 10, 100, 1000 or 5000 pounds is used to determine the quantity of a hazardous substance for which notification is required in the event of a release as specified by CERCLA based on chronic toxicity. Existing data are insufficient to determine an RQ value.

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# HEALTH AND ENVIRONMENTAL EFFECTS PROFILE FOR N,N-DIETHYLANILINE

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## PREFACE

Health and Environmental Effects Profiles (HEEPs) are prepared for the Office of Solid Waste and Emergency Response by the Office of Health and Environmental Assessment. The HEEPs are intended to support listings of hazardous constituents of a wide range of waste streams under Section 3001 of the Resource Conservation and Recovery Act (RCRA), as well as to provide health-related limits for emergency actions under Section 101 of the Comprehensive Environmental Response, Compensation and Liability Act (CERCLA). Both published literature and information obtained from Agency program office files are evaluated as they pertain to potential human health, aquatic life and environmental effects of hazardous waste constituents. The literature searched and the dates of the searches are included in the section titled "Appendix: Literature Searched." The literature search material is current through November, 1985.

Quantitative estimates are presented provided sufficient data are available. For systemic toxicants, these include Reference doses (RfDs) for chronic exposures. An RfD is defined as the amount of a chemical to which humans can be exposed on a daily basis over an extended period of time (usually a lifetime) without suffering a deleterious effect. In the case of suspected carcinogens, RfDs are not estimated in this document series. Instead, a carcinogenic potency factor of $q_1^*$ is provided. These potency estimates are derived for both oral and inhalation exposures where possible. In addition, unit risk estimates for air and drinking water are presented based on inhalation and oral data, respectively.

Reportable quantities (RQs) based on both chronic toxicity and carcinogenicity are derived. The RQ is used to determine the quantity of a hazardous substance for which notification is required in the event of a release as specified under CERCLA. These two RQs (chronic toxicity and carcinogenicity) represent two of six scores developed (the remaining four reflect ignitability, reactivity, aquatic toxicity and acute mammalian toxicity).

The first draft of this document was prepared by Syracuse Research Corporation under EPA Contract No. 68-03-3228. The document was subsequently revised after reviews by staff within the Office of Health and Environmental Assessment: Carcinogen Assessment Group, Reproductive Effects Assessment Group, Exposure Assessment Group, and the Environmental Criteria and Assessment Office in Cincinnati.

The HEEPs will become part of the EPA RCRA and CERCLA dockets.

## ACKNOWLEDGEMENTS

The initial draft of this report was prepared by Syracuse Research Corporation under Contract No. 68-03-3228 for U.S. EPA's Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH. Dr. Christopher DeRosa was the Technical Project Monitor and Helen Ball was the Project Officer. The final documents in this series were prepared for the Office of Solid Waste, Washington, DC.

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## EXECUTIVE SUMMARY

N,N-Diethylaniline is a pale yellow liquid at ambient temperature. It is slightly soluble in alcohol, chloroform and ethylether (Northcott, 1978). The solubility of this compound in water has been reported to vary from 83-14,300 mg/ℓ, presumably depending on the pH of the water; at lower pHs, the compound is expected to show higher solubility. As of January 1985, only two companies manufactured this chemical in the United States (SRI, 1985). The recent U.S. production volume of N,N-diethylaniline is not known, but the total U.S. production was ~2 million pounds in 1976 (Bannister et al., 1979). It is prepared by heating aniline hydrochloride with excess ethanol at 180°C under pressure (Hawley, 1981). N,N-Diethylaniline is used in organic synthesis and in the manufacture of triphenylmethane and thiazine dyes (Kouris and Northcott, 1963).

Information regarding the fate and transport of N,N-diethylaniline in air, water and soil is limited. Based on the available data, only qualitative estimates about some of the fate and transport processes can be made. In water, clay-catalyzed free-radical reaction and photolysis are likely to be significant fate processes (Dragun and Helling, 1985; McKellar, 1967) These two reactions are significant only in water with pH <7. When the pH of the water is >7, these processes may not be significant and evaporation may play a more important role in the loss of the compound from water. Significant bioconcentration of N,N-diethylaniline in aquatic organisms is unlikely (Kawasaki, 1980). The oxidation of N,N-diethylaniline with •OH may be the most significant reaction in the atmosphere. Based on the half-lives of similar aromatic amines (Atkinson, 1985), the half-life of this reaction is expected to be a few hours. In aerobic soils, free radical

oxidation is expected to be the dominant fate process for this chemical (Dragun and Helling, 1985). In acidic soils, the probability of volatilization is expected to be low, and the probability of leaching is expected to be significant in anaerobic soil. In basic soils, these probabilities are expected to be reversed.

Monitoring data on the level of N,N-diethylaniline in the environment are extremely limited. No data on the level of this compound in air or foods were located in the literature. This compound has been detected in surface water in the United States and in Europe at a maximum concentration of 3 µg/ℓ (Ewing et al., 1977; Meijers and Van der Leer, 1976; Piet and Mora, 1983). It was also detected, but not quantified, in one effluent sample from an advanced water treatment plant in Orange County, CA (Lucas, 1984a,b) and in the process water from oil shale retorting operations at a concentration of 2 mg/ℓ (Dobson et al., 1985). N,N-Diethylaniline has not been detected in drinking water in the United States or in Europe (Lucas, 1984a,b; Piet and Mora, 1983).

The only information available concerning toxicity of N,N-diethylaniline to aquatic organisms was provided by Tonogai et al. (1982), who reported 24- and 48-hour $LC_{50}$ values of 40 and 25 mg/ℓ, respectively, for the medaka, Oryzias latipes.

Quantitative pharmacokinetic data on N,N-diethylaniline were not located in the available literature as cited in the Appendix. Laass (1973a) reported that the absorption of N,N-diethylaniline was enhanced in rats simultaneously treated with castor oil. Horn (1937) identified p-diethylaminophenol in the urine of rabbits and dogs treated with N,N-diethylaniline and N,N-diethylaniline-N-oxide.

Pertinent data regarding the carcinogenicity, mutagenicity, teratogenicity, reproductive effects, and chronic and subchronic toxicity of N,N-diethylaniline could not be located in the available literature as cited in the Appendix. Negative results in Salmonella (NTP, 1985) constitute the only data on mutagenicity of N,N-diethylaniline. Although N,N-diethylaniline is expected to cause hematological effects because of its similarity to N,N-dimethylaniline, Jodynis et al. (1977) indicated that N,N-diethylaniline was minimally effective in causing methemoglobinemia in rats. Mixture of N,N-diethylaniline paraffin (Laass, 1973b) enhances the toxicity of N,N-diethylaniline.

Data were insufficient to derive quantitative risk criteria for N,N-diethylaniline. This chemical is classified in IARC Group 3 and EPA Group D, meaning that available data are insufficient to assess the potential carcinogenicity of this compound.

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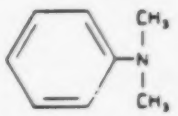
## LIST OF ABBREVIATIONS

| | |
|---|---|
| BCF | Bioconcentration factor |
| CAS | Chemical Abstract Service |
| $K_{oc}$ | Soil sorption coefficient standardized with respect to organic carbon |
| $K_{ow}$ | Octanol/water partition coefficient |
| $LC_{50}$ | Median lethal concentration |
| $LD_{50}$ | Median lethal dose |
| MED | Minimum effective dose |
| ppm | Parts per million |
| RQ | Reportable quantity |

# 1. INTRODUCTION

## 1.1. STRUCTURE AND CAS NUMBER

The chemical commonly called N,N-diethylaniline is also known as benzenamine, N,N-diethyl; aniline, N,N-diethyl; diethylaniline; diethylphenylamine; DEA; N,N-diethylaminobenzene; and phenyldiethylamine (SANSS, 1986). The structure, empirical formula, molecular weight and the CAS Registry number for this chemical are as follows:



Empirical formula: $C_{10}H_{15}N$

Molecular weight: 149.23

CAS Registry number: 91-66-7

## 1.2. PHYSICAL AND CHEMICAL PROPERTIES

N,N-Diethylaniline is a pale yellow liquid at ambient temperature. It is slightly soluble in alcohol, chloroform and ethyl ether (Northcott, 1978). The water solubility values reported for this chemical in the literature vary greatly. Since N,N-diethylaniline is a base with a pKa of 6.57 (Perrin, 1972), its solubility is expected to increase at pH <6.6 (i.e., the solubility is expected to vary with the pH of the water). None of the water solubility data given below specified the pH of the water used. Therefore, the large variation in the solubility values may be entirely or partly due to the differences in the pH of the water used. Some of the physical properties of N,N-diethylaniline are listed below.

| | | |
|---|---|---|
| Melting point: | -38.8°C | Northcott, 1978 |
| Boiling point: | 215-216°C | Northcott, 1978 |
| Density: | 0.935 at 20/40°C | Northcott, 1978 |

| | | |
|---|---|---|
| pKa: | 6.57 | Perrin, 1972 |
| Flash point: | 85°C | Hawley, 1981 |
| Vapor pressure: (estimated) | 0.13 mm Hg at 25°C | Chao et al., 1983 |
| Water solubility: | 14,286 mg/ℓ at 12°C | Northcott, 1978; Windholz, 1983 |
| | 83.2 mg/ℓ at 25°C | Dragun and Helling, 1985 |
| Log $K_{ow}$: | 3.31 (recommended) | Hansch and Leo, 1985 |

The solubility of this compound can also be estimated from its recommended $K_{ow}$ value (Hansch and Leo, 1985) and the regression equation log S = -0.922 log $K_{ow}$ + 4.184 (Lyman et al., 1982). Based on this equation, the solubility of N,N-diethylaniline in water can be estimated to be 14 mg/ℓ, a value several orders of magnitude lower than the value reported by Northcott (1978) and Windholz (1983).

N,N-Diethylaniline is a tertiary amine, which is less reactive than a primary amine; however, it does undergo electrophilic substitution reactions (Gutsche and Pasto, 1975). Oxidation is an environmentally significant reaction of N,N-diethylaniline (Dragun and Helling, 1985) (Chapter 2).

## 1.3. PRODUCTION DATA

The TSCA Inventory (U.S. EPA, 1977) listed nine U.S. companies as producers/importers of this compound in 1977. The total U.S. production of this chemical in 1976 was 1.99 million pounds (Bannister et al., 1979). As of January 1985, Buffalo Color Corp., Buffalo, NY, and DuPont Co., Deepwater, NJ, manufactured the chemical in the United States.

Although the recent U.S. production volume for N,N-diethylaniline is not available, the TSCA Inventory (U.S. EPA, 1977) indicates that Buffalo Color Corp. produced between 0.1 and 1.0 million pounds of this chemical in 1977. N,N-Diethylaniline is prepared by heating aniline hydrochloride with excess ethanol at 180°C under pressure (Hawley, 1981).

## 1.4. USE DATA

N-N-Diethylaniline is used in organic synthesis and in the preparation of triphenylmethane dyes including Basic Green 1, Acid Blue 1 and Basic Violet 4. It is also used in the production of the thiazine dye Basic Blue 25 (Kouris and Northcott, 1963).

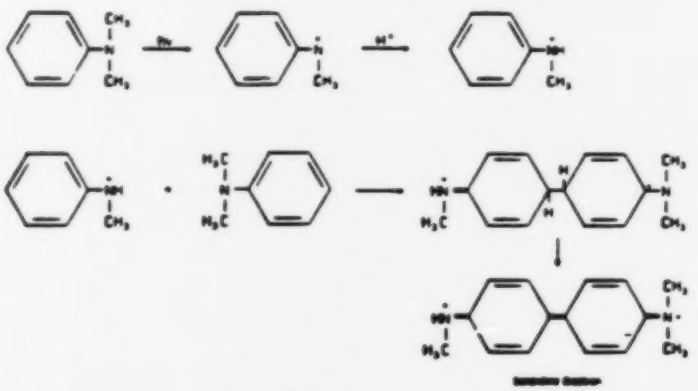
## 1.5. SUMMARY

N,N-Diethylaniline is a pale yellow liquid at ambient temperature. It is slightly soluble in alcohol, chloroform and ethylether (Northcott, 1978). The solubility of this compound in water has been reported to vary from 83-14,300 mg/ℓ, presumably depending on the pH of the water; at lower pHs, the compound is expected to show higher solubility. As of January 1985, only two companies manufactured this chemical in the United States (SRI, 1985). The recent U.S. production volume of N,N-diethylaniline is not known, but the total U.S. production was ~2 million pounds in 1976 (Bannister et al., 1979). It is prepared by heating aniline hydrochloride with excess ethanol at 180°C under pressure (Hawley, 1981). N,N-Diethylaniline is used in organic synthesis and in the manufacture of triphenylmethane and thiazine dyes (Kouris and Northcott, 1963).

## 2. ENVIRONMENTAL FATE AND TRANSPORT PROCESSES

### 2.1. WATER

Little information regarding the fate and transport of N,N-diethylaniline in water could be located in the available literature. N,N-Diethylaniline solution in isooctane has an absorption maximum at 303 nm with an extinction coefficient of $2.37 \times 10^3$ (Windholz, 1983), indicating that this compound will probably undergo photolysis in sunlight. The photolysis of N,N-diethylaniline in air-saturated aqueous solution was studied by McKellar (1967). When $1 \times 10^{-2}$ mol $\ell^{-1}$ of the compound was irradiated by flash photolysis, a colored benzidine divalent cation was formed. The color of the divalent cation was pH dependent; at pH 4.6, the divalent cation was yellow; at pH 5.2, it was green; and at pH 6.3, it was brown. The reaction mechanism was reported to be the following (McKellar, 1967):



This study was conducted with high intensity light (flash photolysis) and the wavelength used was not stated. Although N,N-diethylaniline was not studied, similar effects were induced by sunlight in related compounds in the pH region 2-6.5 (McKellar, 1967). Therefore, it is likely that N,N-diethylaniline will undergo direct photolysis at pH <7, although no quantitative value for the lifetime of this reaction can be estimated.

It would be expected that the photolytically-induced dimerization reaction of N,N-diethylaniline to a benzidine analog would become less favored as the concentration of N,N-diethylaniline decreased.

The biodegradation potential for N,N-diethylaniline was studied by several investigators. Using sewage as microbial inoculum and the standard dilution technique, no degradation of an unspecified concentration of this compound was observed after 5 days of incubation (Heukelekian and Rand, 1955). Using the Japanese MITI test conditions that involves incubating 100 mg/ℓ of test substance with activated sludge for 2 weeks at 25°C, both Kitano (1978) and Kawasaki (1980) reported that this compound is degradation-resistant. Therefore, it appears that N,N-diethylaniline will not significantly biodegrade in natural aquatic systems.

A potential environmental reaction of N,N-diethylaniline at high concentrations is its clay-catalyzed free-radical reaction (i.e., $RO_2\cdot$) to form a benzidine divalent cation (Dragun and Helling, 1985). Hauser and Leagett (1940) found that N,N-diethylaniline underwent a color reaction when mixed with clay. This reaction may occur in natural water containing suspended clay particles; however, no quantitative estimate of the rate of this reaction is available that will permit estimation of the half-life of this compound from the free radical reaction. The direct oxidation of this compound with molecular oxygen present in water may be a significant reaction, but no information was available in the literature.

The removal of N,N-diethylaniline from aquatic systems through physical processes such as volatilization and sorption followed by sedimentation can be qualitatively estimated from its physical properties. In water of pH <7, the solubility of this compound is expected to be high, and since the estimated vapor pressure of N,N-diethylaniline is 0.13 mm Hg (see Section 1.2.),

volatilization will not be significant. At pH >7, however, the value for Henry's Law constant can be estimated to be $3.07 \times 10^{-4}$ atmos-$m^3 mol^{-1}$ based on an aqueous solubility of 83.2 mg/ℓ. Such a value for Henry's Law constant (Lyman et al., 1982) indicates that N,N-diethylaniline is susceptible to volatilization from water of pH >7. The estimated $K_{oc}$ value for diethylaniline is 120 (Kenaga, 1980). Therefore, the removal of this compound through sorption and subsequent precipitation may not be significant.

Using a Japanese MITI test with a flowthrough system (Kitano, 1978), Kawasaki (1980) determined a BCF of <100 for N,N-diethylamine in fish. The BCF can also be estimated from the equation, log BCF = 0.76 log $K_{ow}$ - 0.23 (Lyman et al., 1982). Assuming a log $K_{ow}$ value of 3.31 (see Section 1.2.), the BCF is estimated as 193. Even under conditions of low aqueous solubility, bioaccumulation is not significant. Therefore, significant bioconcentration of N,N-diethylaniline in aquatic organism is not likely.

## 2.2. AIR

Pertinent data regarding the environmental fate and transport of N,N-diethylaniline in air could not be located in the available literature as cited in the Appendix. As stated in Section 2.1., N,N-diethylaniline may undergo photolysis; however, because of the faster rate, oxidation of N,N-diethylaniline by •OH in the atmosphere will be the dominant fate process. Based on the half-lives of aromatic amines, including N,N-dimethylaniline (Atkinson, 1985), the half-life of this reaction is expected to be a few hours.

## 2.3. SOIL

The soil-catalyzed free-radical oxidation of N,N-diethylaniline is expected to be the dominant fate process for this compound (Dragun and Helling, 1985); however, since rate constants or other relevant data for

this reaction are not available, it is not possible to estimate its half-life. Considering the improbability of biodegradation in water (see Section 2.1.), it is also unlikely that biodegradation will be a significant process in soil. Photolysis may occur on soil surfaces, but the significance of this process cannot be predicted.

The possibility of loss of N,N-diethylaniline from soil through volatilization and sorption, and transport through leaching have not been studied. Given the $K_{oc}$ value for N,N-diethylaniline in soil as <200 (see Section 2.1.) and the water solubility of 14,286 mg/ℓ (see Section 1.2.), significant leaching from acidic soil under anaerobic conditions is expected. Under aerobic soil conditions, oxidation is expected to be too rapid to permit significant leaching of the unaltered compound. Qualitative predictions about the volatility of N,N-diethylaniline from soil can be made from its volatility from water (see Section 2.1.). In basic soils, some volatilization of this compound may occur, but the probability of volatilization will be greatly reduced in acidic soils and the probability will decrease incrementally with the lowering of soil pH.

## 2.4. SUMMARY

Information regarding the fate and transport of N,N-diethylaniline in air, water and soil is limited. Based on the available data, only qualitative estimates about some of the fate and transport processes can be made. In water, clay-catalyzed free-radical reaction and photolysis are likely to be significant fate processes (Dragun and Helling, 1985; McKellar, 1967) These two reactions are significant only in water with pH <7. When the pH of the water is >7, these processes may not be significant and evaporation may play a more important role in the loss of the compound from water.

Significant bioconcentration of N,N-diethylaniline in aquatic organisms is unlikely (Kawasaki, 1980). The oxidation of N,N-diethylaniline with •OH may be the most significant reaction in the atmosphere. Based on the half-lives of similar aromatic amines (Atkinson, 1985), the half-life of this reaction is expected to be a few hours. In aerobic soils, free radical oxidation is expected to be the dominant fate process for this chemical (Dragun and Helling, 1985). In acidic soils, the probability of volatilization is expected to be low, and the probability of leaching is expected to be significant in anaerobic soil. In basic soils, these probabilities are expected to be reversed.

## 3. EXPOSURE

### 3.1. WATER

N,N-Diethylaniline was detected at a concentration of 2 mg/ℓ in the process water from oil shale retorting operations in Rundle, Australia (Dobson et al., 1985) and at an unspecified concentration in water from the River Waal at Brakel, the Netherlands (Meijers and Van der Leer, 1976). In the Netherlands, the level of N,N-diethylaniline in Rhine River water was reported to be 1 µg/ℓ, but this compound was not detected in tap water (Piet and Mora, 1983).

Several sites on the Mississippi River Basin from Alabama to Texas were monitored for N,N-diethylaniline (Ewing et al., 1977; U.S. EPA, 1986a); it was detected in only 1/204 samples at a concentration of 3 µg/ℓ. Seventeen drinking water samples from 7 states and 16 samples of advanced water treatment effluents from 3 states were monitored for the presence of organic compounds (Lucas, 1984a,b). N,N-Diethylaniline was not detected in any drinking water samples, and this compound was tentatively identified in only one advanced water treatment sample from Orange County, CA (Lucas, 1984a,b).

### 3.2. AIR

Pertinent data regarding the monitoring of N,N-diethylaniline in air could not be located in the available literature as cited in the Appendix.

### 3.3. FOODS

Pertinent data regarding levels of N,N-diethylaniline in food could not be located in the available literature as cited in the Appendix.

### 3.4. SUMMARY

Monitoring data on the level of N,N-diethylaniline in the environment are extremely limited. No data on the level of this compound in air or

foods were located in the literature. This compound has been detected in surface water in the United States and in Europe at a maximum concentration of 3 µg/ℓ (Ewing et al., 1977; Meijers and Van der Leer, 1976; Piet and Mora, 1983). It was also detected, but not quantified, in one effluent sample from an advanced water treatment plant in Orange County, CA (Lucas, 1984a,b) and in the process water from oil shale retorting operations at a concentration of 2 mg/ℓ (Dobson et al., 1985). N,N-Diethylaniline has not been detected in drinking water in the United States or in Europe (Lucas, 1984a,b; Piet and Mora, 1983).

## 4. PHARMACOKINETICS

### 4.1. ABSORPTION

Pertinent data regarding the absorption of N,N-diethylaniline could not be located in the available literature as cited in the Appendix.

### 4.2. DISTRIBUTION

Pertinent data regarding the distribution of N.N-diethylaniline could not be located in the available literature as cited in the Appendix.

### 4.3. METABOLISM

Pertinent data regarding the metabolism of N.N-diethylaniline could not be located in the available literature as cited in the Appendix.

### 4.4. EXCRETION

Pertinent data regarding the excretion of N.N-diethylaniline could not be located in the available literature as cited in the Appendix; however, Horn (1937) reported that p-diethylaminophenol was identified in the urine of rabbits and dogs after oral administration of N,N-diethylaniline and N,N-diethylaniline-N-oxide.

### 4.5. SUMMARY

Quantitative pharmacokinetic data on N,N-diethylaniline could not be located in the available literature as cited in the Appendix. Laass (1973a) reported that the absorption of N,N-diethylaniline was enhanced in rats simultaneously treated with castor oil. Horn (1937) identified p-diethylaminophenol in the urine of rabbits and dogs treated with N,N-diethylaniline and N,N-diethylaniline-N-oxide.

# 5. EFFECTS

## 5.1. CARCINOGENICITY

Pertinent data regarding the carcinogenicity of N,N-diethylaniline could not be located in the available literature as cited in the Appendix, and this chemical is not scheduled for testing by the National Toxicology Program (NTP, 1986).

## 5.2. MUTAGENICITY

While pertinent data regarding the mutagenicity of N,N-diethylaniline could not be located in the available literature as cited in the Appendix, N,N-diethylaniline was found negative in Salmonella tests conducted by NTP (1985).

## 5.3. TERATOGENICITY

Pertinent data regarding the teratogenicity of N,N-diethylaniline could not be located in the available literature as cited in the Appendix.

## 5.4. OTHER REPRODUCTIVE EFFECTS

Pertinent data regarding reproductive effects of N,N-diethylaniline could not be located in the available literature as cited in the Appendix.

## 5.5. CHRONIC AND SUBCHRONIC TOXICITY

Pertinent data regarding the chronic and subchronic toxicity of N,N-diethylaniline could not be located in the available literature as cited in the Appendix.

## 5.6. OTHER RELEVANT INFORMATION

The $LD_{50}$ and $LC_{50}$ values for N,N-diethylaniline are listed in Table 5-1. Based on the similarity between the structure of N,N-diethylaniline and N,N-dimethylaniline, N,N-diethylaniline is expected to cause methemoglobinemia and other pathological changes similar to the effects caused by N,N-dimethylaniline (Voss et al., 1981). Jodynis et al. (1977) indicated,

TABLE 5-1

$LD_{50}$ and $LC_{50}$ Values for N,N-Diethylaniline

| Route | Species | $LD_{50}/LC_{50}$ | Reference |
|---|---|---|---|
| Oral | rat | 782 mg/kg | NIOSH, 1986 |
| Inhalation | rat | 1920 mg/m³ | Voss et al., 1981 |
| Intraperitoneal | rat | 420 mg/kg | NIOSH, 1986 |

NR = Not reported

however, that N,N-diethylaniline was not very effective in causing methemoglobinemia in rats. Kiese et al. (1966) found that the methemoglobin level in the blood of dogs rose rapidly following an intravenous dose of 0.6 mmol/kg N,N-diethylaniline hydrochloride or N,N-dimethylaniline hydrochloride. N,N-diethylaniline-N-oxide, a metabolite of N,N-diethylaniline, was much less potent than the N-oxide of N,N-dimethylaniline in producing methemoglobin after intravenous injection.

Pollevka et al. (1976) reported that the insect repellent activity of N,N-diethylaniline was enhanced after mixture with polyhydroxy compounds, such as polyethylene glycol.

## 5.7. SUMMARY

Pertinent data regarding the carcinogenicity, mutagenicity, teratogenicity, reproductive effects, and chronic and subchronic toxicity of N,N-diethylaniline could not be located in the available literature as cited in the Appendix. Negative results in Salmonella (NTP, 1985) constitute the only data on mutagenicity of N,N-diethylaniline. Although N,N-diethylaniline is expected to cause hematological effects because of its similarity to N,N-dimethylaniline, Jodynis et al. (1977) indicated that N,N-diethylaniline was minimally effective in causing methemoglobinemia in rats. Mixture of N,N-diethylaniline paraffin (Laass, 1973b) enhances the toxicity of N,N-diethylaniline.

## 6. AQUATIC TOXICITY

### 6.1. ACUTE

In the only study available, Tonogai et al. (1982) reported 24- and 48-hour $LC_{50}$ values of 40 and 25 mg/ℓ for the medaka, Oryzias latipes.

### 6.2. CHRONIC

Pertinent data regarding chronic toxicity of N,N-diethylaniline to aquatic organisms could not be located in the available literature as cited in the Appendix.

### 6.3. PLANTS

Pertinent data regarding effects of N,N-diethylaniline on aquatic plants could not be located in the available literature as cited in the Appendix.

### 6.4. RESIDUES

Pertinent data regarding N,N-diethylaniline residues in aquatic biota could not be located in the available literature as cited in the Appendix.

### 6.5. SUMMARY

The only information available concerning toxicity of N,N-diethylaniline to aquatic organisms was provided by Tonogai et al. (1982), who reported 24- and 48-hour $LC_{50}$ values of 40 and 25 mg/ℓ, respectively, for the medaka, Oryzias latipes.

## 7. EXISTING GUIDELINES AND STANDARDS

### 7.1. HUMAN

Pertinent guidelines and standards, including EPA ambient water and air quality criteria, drinking water standards, FAO/WHO ADIs, EPA or FDA tolerances for raw agricultural commodities or foods, and ACGIH, NIOSH or OSHA occupational exposure limits could not be located in the available literature as cited in the Appendix.

### 7.2. AQUATIC

Guidelines and standards for the protection of aquatic biota from the effects of N,N-diethylaniline could not be located in the available literature as cited in the Appendix.

## 8. RISK ASSESSMENT

Because of the lack of information on the carcinogenicity, developmental and reproductive effects and systemic toxicity after subchronic or chronic ingestion or inhalation of N,N-diethylaniline, it is not possible to perform a quantitative risk assessment on N,N-diethylaniline at this time.

## 9. REPORTABLE QUANTITIES

### 9.1. REPORTABLE QUANTITY (RQ) RANKING BASED ON CHRONIC TOXICITY

There are insufficient data available on N,N-diethylaniline to derive an RQ (Table 9-1).

### 9.2. WEIGHT OF EVIDENCE AND POTENCY FACTOR ($F=1/ED_{10}$) FOR CARCINOGENICITY

Pertinent data regarding the carcinogenicity of N,N-diethylaniline to animals or humans could not be located in the available literature as cited in the Appendix. Therefore, N,N-diethylaniline is a Group 3 chemical according to the classification scheme of IARC and a Group D chemical according to the classification scheme of EPA (U.S. EPA, 1986b).

TABLE 9-1

N,N-Diethylaniline

Minimum Effective Dose (MED) and Reportable Quantity (RQ)

| | |
|---|---|
| Route: | |
| Dose: | |
| Effect: | |
| Reference: | |
| RV: | |
| $RV_d$: | |
| $RV_e$: | |
| Composite Score: | |
| RQ: | Data are not sufficient for deriving an RQ |

## 10. REFERENCES


Atkinson, R. 1985. Kinetics and mechanisms of the gas phase reactions of the hydroxyl radical with organic compounds under atmospheric conditions. Chem. Rev. 85: 69-201.

Bannister, D.W., A.D. Olin and H.A. Stingl. 1979. In: Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 8, 3rd ed., M. Grayson and D. Eckroth, Ed. John Wiley and Sons, New York. p. 174.

Chao, J., C.T. Lin and T.H. Chung. 1983. Vapor pressure of coal chemicals. J. Phys. Chem. Ref. Data. 12: 1033-1063.

Dobson, K.R., M. Stephenson, P.F. Greenfield and P.R.F. Bell. 1985. Identification and treatability of organics in oil shale retort water. Water Res. 19: 849-856.

Dragun, J. and C.S. Helling. 1985. Physicochemical and structural relationships of organic chemicals undergoing soil- and clay-catalyzed free-radical oxidation. Soil Sci. 139: 100-111.

Ewing, B.B, S.K. Chian, J.C. Cook et al. 1977. Monitoring to Detect Previously Unrecognized Pollutants in Surface Waters. Appendix: Organic Analysis Data. EPA-560/6-77-015. (Appendix: EPA-560/6-77-015A) 170 p.

Gutsche, C.D. and D.J. Pasto. 1975. Fundamentals of Organic Chemistry. Prentice Hall, Inc., Englewood Cliffs, NJ. p. 317.

Hansch, C. and A.J. Leo. 1985. Medchem Project. Issue No. 26. Pomona College, Claremont, CA.

Hauser, E.A. and M.B. Legett. 1940. Color reactions between clays and amines. J. Am. Chem. Soc. 62: 1811-1814.

Hawley, G.G. 1981. The Condensed Chemical Dictionary, 10th ed. Van Nostrand Reinhold Co., New York. p. 344

Heukelekian, H. and M.C. Rand. 1955. Biochemical oxygen demand of pure organic compounds. J. Water Pollut. Control Assoc. 29: 1040-1053.

Horn, F. 1937. Uber den abbau des Diathylanilins and Diathylanilinoxydo im Terkorper. Hoppe - Seylers Z. Physiol. Chem. 249: 82. (Ger.) (Cited in Kiese et al., 1966)

Jodynis, J., W. Mlynarczyk, E. Szopska and W. Szopski. 1977. Effect of the chemical structure of some aromatic compounds on methemoslobin-formins properties. Bromatol. Chem. Toksykol. 10(2): 151-155. (CA 87:178513d)

Kawasaki, M. 1980. Experiences with the test scheme under the Chemical Control Law of Japan: An approach to structure-activity correlations. Ecotoxicol. Environ. Saf. 4: 444-454.

Kenaga, E.E. 1980. Predicted bioconcentration factors and soil sorption coefficients of pesticides and other chemicals. Ecotoxicol. Environ. Saf. 4: 26-38.

Kiese, M., E. Rauscher and N. Weger. 1966. The role of N,N-dimethylaniline-N-oxide in the formation of hemoglobin following the absorption of N,N-dimethylaniline. Naunyn - Schmiedebergs Arch. Pharmak. u. exp. Path. 254: 253-260.

Kitano, M. 1978. Biodegradation and Bioaccumulation Test on Chemical Substances. OECD Tokyo Meeting. Reference Book TSU-No. 3.

Kouris, C.S. and J. Northcott. 1963. Aniline and its derivatives. In: Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 2, 2nd ed., M. Grayson and D. Eckroth, Ed. John Wiley and Sons, New York. p. 411-427.

Laass, W. 1973a. Castor oil in the treatment of acute oral intoxication with organic solvents. Pharmazie. 28(10): 684-685.

Laass, W. 1973b. Suitability of liquid paraffin in the treatment of acute oral poisons with organic solvents. Pharmazie. 28(1): 65-66.

Lucas, S.V. 1984a. GC/MS Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Concentrates: Vol. 1. Analysis results for 17 Drinking Water, 16 Advanced Waste Treatment and 3 Process Blank Concentrates. EPA-600/1-84-020A. NTIS PB85-128221. 303 p.

Lucas, S.V. 1984b. GC/MS Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Concentrates: Vol. 2. Computer Printed Tabulations of Compound Identification Results for Large-Volume Concentrations. EPA-600/1-84-020B. NTIS PB85-128239. 382 p.

Lyman, W.J., W.F. Reehl and D.H. Rosenblatt. 1982. Handbook of Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds. McGraw-Hill Book Co., New York. p. 2-14, 4-9, 5-5 and 15-16.

McKellar, J.F. 1967. The photooxidation of simple N-alkyl anilines studied by flash photolysis. Photochem. Photobiol. 6: 287-299.

Meijers, A.P. and R.C. Van der Leer. 1976. The occurrence of organic micropollutants in the River Rhine and the River Maas in 1974. Water Res. 10(7): 597-604.

NIOSH (National Institute for Occupational Safety and Health). 1986. Registry of Toxic Effects of Chemical Substances. Online.

Northcott, J. 1978. Aniline and its derivatives. In: Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 2, 3rd ed., M. Grayson and D. Eckroth, Ed. John Wiley and Sons, New York. p. 317

NTP (National Toxicology Program). 1985. Results and Status on all NTP Chemicals. 8/28/85.

NTP (National Toxicology Program). 1986. Management Status Report. 3/12/86.

Perrin, D.D. 1972. Dissociation Constants of Organic Bases in Aqueous Solution. IUPAC Chemical Data Services: Supplement 1972. Butterworth, London.

Piet, G.J. and C.F. Morra. 1983. Behavior of organic micropollutants during underground passage. In: Artificial Groundwater Recharge (Water Resources Engineering Series), L. Huisman and T.N. Olsthorn, Ed. Pitman Publ., Marshfield, MA. p. 31-42.

Pollevka, M., E. Machova and A. Puma. 1976. Insect repellent. Czech. PATENT NO. 163571. (CA 86:12715a)

SANSS (Structure and Nomenclature Search System). 1986. Chemical Information Systems, Inc., Baltimore, MD. Online.

SRI (Stanford Research Institute). 1985. Directory of Chemical Producers. United States of America. SRI International, Menlo Park, CA. p. 525.

Tonogai, Y., S. Osawa, Y. Ito and M. Iwaida. 1982. Actual survey on TLm (mediam tolerance limit) value of environmental pollutants, especially on amines, nitriles, aromatic nitrosen compounds and artificial dyes. J. Toxicol. Sci. 7(3): 193-203.

U.S. EPA. 1977. Computer print-out of non-confidential production data from TSCA inventory. OPTS, CID, U.S. EPA, Washington, DC.

U.S. EPA. 1986a. STORET Water Quality Database. Online: April, 1986.

U.S. EPA. 1986b. Guidelines for Carcinogen Risk Assessment. Federal Register. 51(185): 33992-34003.

Voss, K.A., P.J. Becci and R.A. Parent. 1981. Acute $LC_{50}$ of diethylaniline in Sprague-Dawley rats. Food and Drug Research Laboratories, Inc. Study No. 6771 for Buffalo Color Corp., West Paterson, NJ. TSCA 8(e)submission. Document No. 88-8100369 8eHQ-0482-0430, Microfiche No. OTS 0505450.

Windholz, M., Ed. 1983. The Merck Index. An Encyclopedia of Chemicals, Drugs, and Biologicals, 10th ed. Merck and Co., Inc., Rahway, NJ. p. 452.

## APPENDIX

## LITERATURE SEARCHED

This profile is based on data identified by computerized literature searches of the following:

GLOBAL
TSCATS
CASR online (U.S. EPA Chemical Activities Status Report)
CAS online STN International
TOXLINE
TOXBACK 76
TOXBACK 65
RTECS
OHM TADS
STORET
SRC Environmental Fate Data Bases
SANSS
AQUIRE
TSCAPP
NTIS
Federal Register

These searches were conducted in April, 1986. In addition, hand searches were made of Chemical Abstracts (Collective Indices 6 and 7), and the following secondary sources were reviewed:

ACGIH (American Conference of Governmental Industrial Hygienists). 1986. Documentation of the Threshold Limit Values and Biological Exposure Indices, 5th ed. Cincinnati, OH.

ACGIH (American Conference of Governmental Industrial Hygienists). 1986. TLVs: Threshold Limit Values for Chemical Substances and Physical Agents in the Workroom Environment with Intended Changes for 1985-1986. Cincinnati, OH. 114 p.

Clayton, G.D. and F.E. Clayton, Ed. 1981. Patty's Industrial Hygiene and Toxicology, 3rd rev. ed., Vol. 2A. John Wiley and Sons, NY. 2878 p.

Clayton, G.D. and F.E. Clayton, Ed. 1981. Patty's Industrial Hygiene and Toxicology, 3rd rev. ed., Vol. 2B. John Wiley and Sons, NY. p. 2879-3816.

Clayton, G.D. and F.E. Clayton, Ed. 1982. Patty's Industrial Hygiene and Toxicology, 3rd rev. ed., Vol. 2C. John Wiley and Sons, NY. p. 3817-5112.

Grayson, M. and D. Eckroth, Ed. 1978-1983. Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed. John Wiley and Sons, NY. 23 Volumes.

Hamilton, A. and H.L. Hardy. 1974. Industrial Toxicology, 3rd ed. Publishing Sciences Group, Inc., Littleton, MA. 575 p.

IARC (International Agency for Research on Cancer). IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans. WHO, IARC, Lyons, France.

Jaber, H.M., W.R. Mabey, S.T. Liu, T.W. Chow and H.L. Johnson. 1984. Data aquisition for environmental transport and fate screening for compounds of interest in the Office of Solid Waste. EPA 600/6-84-010. NTIS PB84-243906. SRI International, Menlo Park, CA.

NTP (National Toxicology Program). 1986. Toxicology Research and Testing Program. Chemicals on Standard Protocol. Management Status.

Ouellette, R.P. and J.A. King. 1977. Chemical Week Pesticide Register. McGraw-Hill Book Co., NY.

Sax, N.I. 1979. Dangerous Properties of Industrial Materials, 5th ed. Van Nostrand Reinhold Co., NY.

SRI (Stanford Research Institute). 1984. Directory of Chemical Producers. Menlo Park, CA.

U.S. EPA. 1986. Report on Status in the Special Review Program, Registration Standard Program and the Data Call in Programs. Office of Pesticide Programs, Washington, DC.

U.S. EPA. 1985. CSB Existing Chemical Assessment Tracking System. Name and CAS Number Ordered Indexes. Office of Toxic Substances, Washington, DC.

USITC (U.S. International Trade Commission). 1985. Synthetic Organic Chemicals. U.S. Production and Sales, 1984, USITC Publ. 1745, Washington, DC.

Verschueren, K. 1983. Handbook of Environmental Data on Organic Chemicals, 2nd ed. Van Nostrand Reinhold Co., NY.

Worthing, C.R. and S.B. Walker, Ed. 1983. The Pesticide Manual. British Crop Protection Council. 695 p.

Windholz, M., Ed. 1983. The Merck Index, 10th ed. Merck and Co., Inc., Rahway, NJ.

In addition, approximately 30 compendia of aquatic toxicity data were reviewed, including the following:


Battelle's Columbus Laboratories. 1971. Water Quality Criteria Data Book. Volume 3. Effects of Chemicals on Aquatic Life. Selected Data from the Literature through 1968. Prepared for the U.S. EPA under Contract No. 68-01-0007. Washington, DC.

Johnson, W.W. and M.T. Finley. 1980. Handbook of Acute Toxicity of Chemicals to Fish and Aquatic Invertebrates. Summaries of Toxicity Tests Conducted at Columbia National Fisheries Research Laboratory. 1965-1978. U.S. Dept. Interior, Fish and Wildlife Serv. Res. Publ. 137, Washington, DC.

McKee, J.E. and H.W. Wolf. 1963. Water Quality Criteria, 2nd ed. Prepared for the Resources Agency of California, State Water Quality Control Board. Publ. No. 3-A.

Pimental, D. 1971. Ecological Effects of Pesticides on Non-Target Species. Prepared for the U.S. EPA, Washington, DC. PB-269605.

Schneider, B.A. 1979. Toxicology Handbook. Mammalian and Aquatic Data. Book 1: Toxicology Data. Office of Pesticide Programs, U.S. EPA, Washington, DC. EPA 540/9-79-003. NTIS PB 80-196876.